does not predict a gap due to the crossover of bands along the Γ-N direction, which could give rise to surface states.

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Piezo-optical Evidence for Λ Transitions at the 3.4-eV Optical Structure of Silicon

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We report the effects of large uniaxial stresses, which produce splittings and shifts large compared to the spin-orbit interaction, along the [001] and [111] direction on the wavelength-modulated reflectivity spectrum of Si in the region around 3.4 eV. Our results are interpreted in terms of both interband and intraband splittings of the orbital bands and indicate conclusively that the optical structure corresponding to the main peak in reflectivity around 3.4 eV is due to Λ_3-Λ_1 (or L_3'-L_1) transitions.

For a number of years there has been considerable controversy concerning the origin of the 3.4-eV optical structure in Si. Both experimental and theoretical evidence have been divided between assignments of the main part of this structure to Δ_5-Δ_1 transitions (along equivalent [001] axes)[1-6] or to Λ_3-Λ_1 transitions (along equivalent [111] axes).[7-13] The main experimental evidence for the Δ assignment has been the original chemical-shift data on Ge-Si alloys,[1] dc[2] and ac[3] piezoreflectivity, and, more recently, a study of uniaxial stress on the wavelength-modulated (WLM) spectra.[5] Doubts concerning the Δ assignment have been raised on the basis of other theoretical[7-11] and experimental work,[12-16] particularly with regard to the hydrostatic-pressure coefficient of this structure. Recent electroreflectance experiments on Si[13] and hydrostatic-pressure investigations of the electroreflectance spectrum of Ge-Si alloys[12] have given strong weight to the Λ assignment. In this Letter we report the effects of uniaxial stresses of up to 23×10^9 dyn cm^{-2} along the [111] and [001] directions on the WLM reflectivity spectrum of Si at 77°K, using light polarized parallel ($\parallel$) and perpendicular ($\perp$) to the stress axis. These large stresses produce splittings and shifts which are large compared to the spin-orbit interaction (44 meV at $\vec{k}=0$) and hence have enabled us to observe new stress-dependent structures and splittings, which are in-

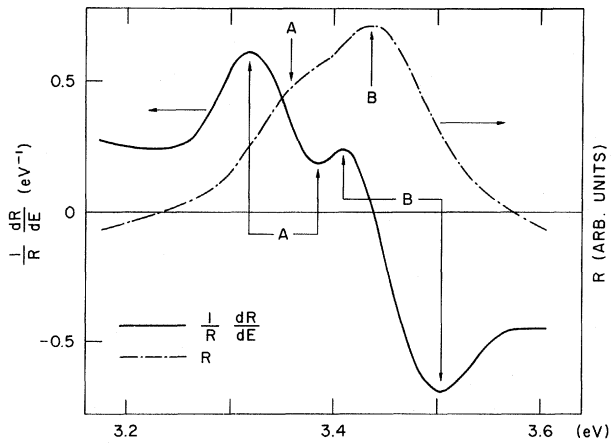

FIG. 1. Wavelength-modulated and reflectivity spectra of Si at 77°K for $X=0$. The peaks and valleys in the wavelength-modulated spectrum, which are indicated by arrows, correspond to inflection points on either side of the respective structure in the reflectance.

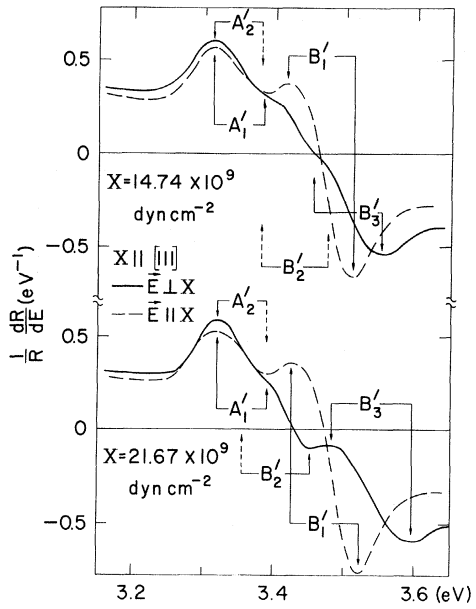

FIG. 2. Wavelength-modulated reflectivity spectrum for $X=14.74\times10^9$ and 21.67×10^9 dyn cm^{-2} along [111]. Arrows with solid lines are used to indicate clearly discernible peaks and/or valleys while arrows with broken lines represent the position of "unresolved" features as discussed in the text. The feature B_2' is well resolved at the highest stress although weak structure associated with it can be seen at the lower stress.

terpreted in terms of both interband and intraband effects (the latter having been neglected by previous authors[2,3,5]). Our conclusions, based on symmetry considerations, indicate clearly that the main component of the 3.4-eV reflectivity peak in Si is due to Λ (or L) transitions. These new observations remove the apparent discrepancy between the areas of experimental evidence for Δ as opposed to Λ symmetry. Thus this structure in Si is analogous to the E_1 peaks (Λ or L transitions) which are characteristic of the other semiconductors of this family.[17-19]

The details of the optical, stress, and cryogenic apparatus have been described elsewhere.[19] The modulation amplitude was 7 Å at 22 Hz.

Figure 1 shows the WLM and reflectivity (R) spectra of Si at 77°K for stress $X=0$. The R spectrum was obtained by integrating the WLM spectrum. The structure in R near 3.4 eV is composed of a strong peak B, and a weaker structure A which appears as a shoulder on the low-energy side of B.[20] The peaks and valleys in the WLM spectrum (indicated by arrows in Fig. 1) correspond to inflection points on either side of the corresponding structure (A or B) in R. Figure 2 shows the WLM spectrum for $X=14.74\times10^9$ and 21.67×10^9 dyn cm^{-2} along [111] for light polarized $\parallel X$ and $\perp X$. The following discussion will concentrate on the stress dependence of those structures in the WLM spectra associated with the main peak in reflectivity B. Application of stress along [111] produces polarization-dependent splittings of this structure. Two sets of structures are observed for the $\perp$ case (labeled B_2' and B_3'), while for the $\parallel$ case only one set of peaks and valleys is seen (B_1'), occurring at an energy between those of B_2' and B_3'.

The determination of the stress dependence of the energies of the B structures is complicated by the facts that (1) B_2' merges with A, and (2) the individual peaks and valleys of B_2' and B_3' are not completely resolved since the stress-induced splitting between them is comparable to their linewidths. In the analysis, we have used the fact that the linewidth of the individual B structures is not stress dependent, i.e., the separation between a peak and valley remains constant. This is clearly indicated by the behavior of B_1' over the entire stress range and by B_3' at high stresses (see Fig. 2). Arrows with solid lines are used to indicate clearly discernible peaks and/or valleys while arrows with dashed lines represent the position of "unresolved" features in the sense discussed above.

The stress dependence of the energies of the A and B structures of the WLM spectra for $X\parallel[111]$ and $X\parallel[001]$ are plotted in Fig. 3. As discussed above, although B_2' is well resolved only at the highest stresses, we have been able to follow weak structure (shoulders in WLM) associated

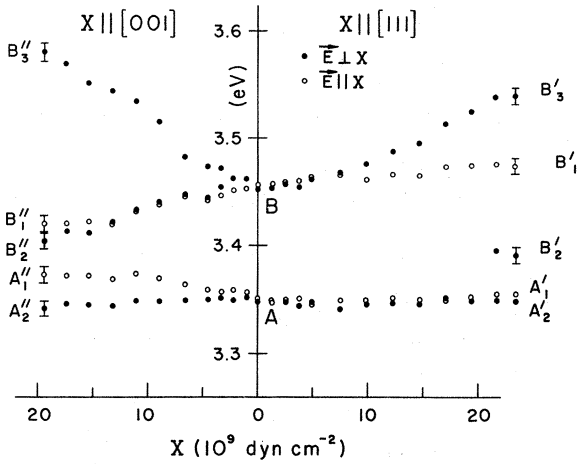

FIG. 3. Stress dependence of the A and B structures of the wavelength-modulated reflectivity spectrum for stress along [001] and [111]. Representative error bars are shown.

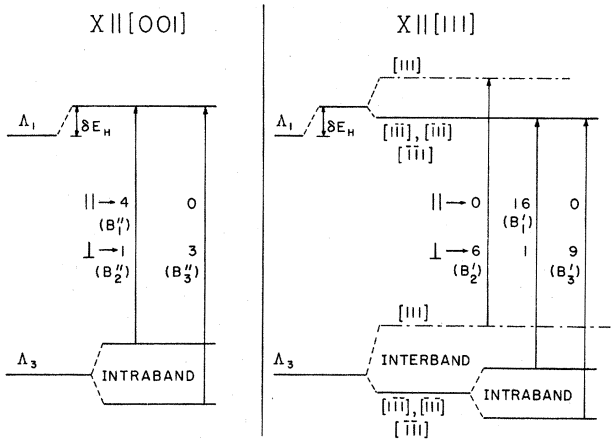

FIG. 4. Schematic representation of the stress-induced interband and intraband splittings of the Λ_3 valence and Λ_1 conduction bands. δE_H represents the effect of the hydrostatic component of the strain on the interband transition. Selection rules and relative intensities have been calculated using the $\vec{k}\cdot\vec{p}$ wave functions of Ref. 14.

with it (see Fig. 2) over a much larger stress region. For $X \leq 10\times10^9$ dyn cm^{-2}, B_1' and B_3' are nearly degenerate and weak structure associated with B_2' has not yet appeared. The A structure for $X\|[111]$ has only a weak stress dependence with the $\|$ (A_1') and $\perp$ (A_2') components remaining degenerate. In the case of $X\|[001]$, two components of the B structure are observed for $\perp$ (B_2'' and B_3''), while one is seen for $\|$ (B_1''). However, in contrast to $X\|[111]$, the low-energy component for $\perp$ is degenerate with the $\|$ component. For this stress direction the A structure exhibits a small stress-induced splitting.

Our results and those of Refs. 2 and 5 are in agreement in the region of stresses they attained ($X \leq 10\times10^9$ dyn cm^{-2}). Thus, the significantly larger stresses we have reached are crucial since they have enabled us to observe new features, i.e., B_2' and the splitting between B_1' and B_3'.

The stress-induced, polarization-dependent splittings and shifts are interpreted in terms of both interband and intraband splittings of the Λ_3-Λ_1 orbital bands.[14,19,21] Only orbital bands will be considered since the stress-induced splittings we have attained are considerably larger than the spin-orbit splitting. In general, for transitions at $\vec{k}\neq 0$, application of stress causes two effects: (1) the removal of the equivalence of the critical points whose $\vec{k}$ vectors do not have equal projections onto the stress direction (interband splitting), and (2) the splitting of doubly degenerate orbital bands whose $\vec{k}$ vectors are not parallel to X (intraband splitting). For $X\|[001]$ (left-hand side, Fig. 4) there is no interband splitting since this stress direction does not remove the degeneracy of the equivalent $\langle 111\rangle$ directions. There is, however, an intraband splitting of the doubly degenerate Λ_3 valence bands. The effect on the Λ_3-Λ_1 transition of the hydrostatic pressure component of the strain is denoted by δE_H. For $X\|[111]$ (right-hand side, Fig. 4), the situation is more complex since both interband and intraband effects are produced: The [111] band is split off from the remaining three bands and there is an intraband splitting of the latter group. The indicated selection rules and relative intensities have been calculated from the appropriate $\vec{k}\cdot\vec{p}$ wave functions of Ref. 14. These selection rules are in agreement with Kane's analysis for the orbital bands along Λ.[21]

Comparison of Figs. 3 and 4 reveals that the above theoretical model accounts for the experimentally observed stress and polarization dependence of the B structures. For $X\|[001]$ two transitions are seen, the low-energy component being allowed for both $\|$ (B_1'') and $\perp$ (B_2''), while the high-energy component is seen only for $\perp$ (B_3''). In the case of the [111] stress there are three transitions, the high (B_3') and low (B_2') energy components being allowed only for $\perp$ while the intermediate energy component (B_1') is predominantly $\|$. Similar considerations of Δ_5-Δ_1, $\Gamma_{25'}$-Γ_{15},[22] or $\Gamma_{25'}$-$\Gamma_{2'}$[23] transitions do not account for the experimental observations.

From the observed stress dependence of the B

structures we determine values for the deformation potentials $D_1^1 = -8 \pm 1$ eV, $D_1^5 = 10 \pm 2$ eV, $D_3^3 = 5 \pm 1$ eV, and $D_3^5 = 4 \pm 1$ eV.[21] We find good agreement between the above value of D_1^1, which describes the effect of hydrostatic strain, and those determined from hydrostatic-pressure measurements.[12,24] The parameter D_1^5 represents the interband splitting created by [111] stress while D_3^3 and D_3^5 are associated with the intraband splitting for $X \parallel [001]$ and [111], respectively. Our value for D_1^5 is comparable to those for the Λ transitions in several semiconductors of this family.[2,19,25,26] Although the values for D_3^3 and D_3^5 for Si are about a factor of 2 larger than those of Ge,[25] they are in agreement with the theoretical calculations of Goroff and Kleinman for Si.[7] The ratio $D_3^5/D_3^3 = 0.8 \pm 0.3$ is comparable to that for Ge[25] and GaAs.[26]

The observed stress dependence of the A structure has not enabled us to make a conclusive symmetry assignment of this spectral feature, as was done for the main reflectivity peak B. A theoretical calculation of the WLM spectrum has attributed the A structure to transitions in a volume centered at $(2\pi/a)(0.3, 0.3, 0.2)$ and to Δ_5-Δ_1 transitions close to Γ.[11] The experimental hydrostatic-pressure coefficient agrees with that of the E_0' peak of Ge,[12] which has been identified as a $\Gamma_{25'}$-Γ_{15} transition in this material.[22] Our results (see Fig. 3) cannot be explained by a $\Gamma_{25'}$-Γ_{15} transition but are not inconsistent with a Δ assignment if it is assumed that the intraband splitting for both [001] and [111] stress is very small.

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